Propane
74-98-6 | DTXSID5026386

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3540 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.71e-01

Confidence level: 7.61e-01

Nearest Neighbors from the Training Set

Image not found
Bromochloromethane
Measured: 7150
Predicted: 198

Image not found
1,3-Butadiyne
Measured: 2010
Predicted: 1030

Image not found
2-Bromopropane
Measured: 2610
Predicted: 182

Image not found
1,2-Dibromoethane
Measured: 1820
Predicted: 19.9

Image not found
2-Methyl-2-propanethiol
Measured: 2540
Predicted: 126